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UCRL-PROC-203257

Electronic Properties of Carbon at Extreme Conditions from ab Initio Simulations

A.A. Correa, S.A. Bonev, G. Galli, R.W. Falcone

March 30, 2004

2004 March American Physical Society Meeting
Montreal, Canada
March 22, 2004 through March 26, 2004

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A. A. Correa[1,2] S. A. Bonev[2] G. Galli[2] R. W. Falcone[1]

[1]Department of Physics
University of California at Berkeley

[2]Lawrence Livermore National Laboratory

APS March meeting, Montreal 2004

Motivation

Why Carbon at extreme conditions?

- **Astrophysics and Planetary Science:** Jovian Planets[1] and White Dwarfs[2]
- **Technology:** High-pressure research, transparency problem[3]

Why *ab initio* simulation?

- **Practical:** Experiments are difficult at extreme conditions and results are controversial.
- **Methodology:** Empirical/non-abinitio simulations gave misleading results[4].

Electronic Gap dependence with Pressure and Temperature

[1] W. B. Hubbard, *Science* **214**, 145-9 (1981)
[2] V. Weidemann *et al.*, *Astron.& Astroph.* **297**(1), 216-222 (1995)
[3] A. L. Ruoff et al., *J. Appl. Phys.* **70**, 2066 (1991)
[4] C. J. Wu *et al.*, *PRL* **89**, 135701 (2002)

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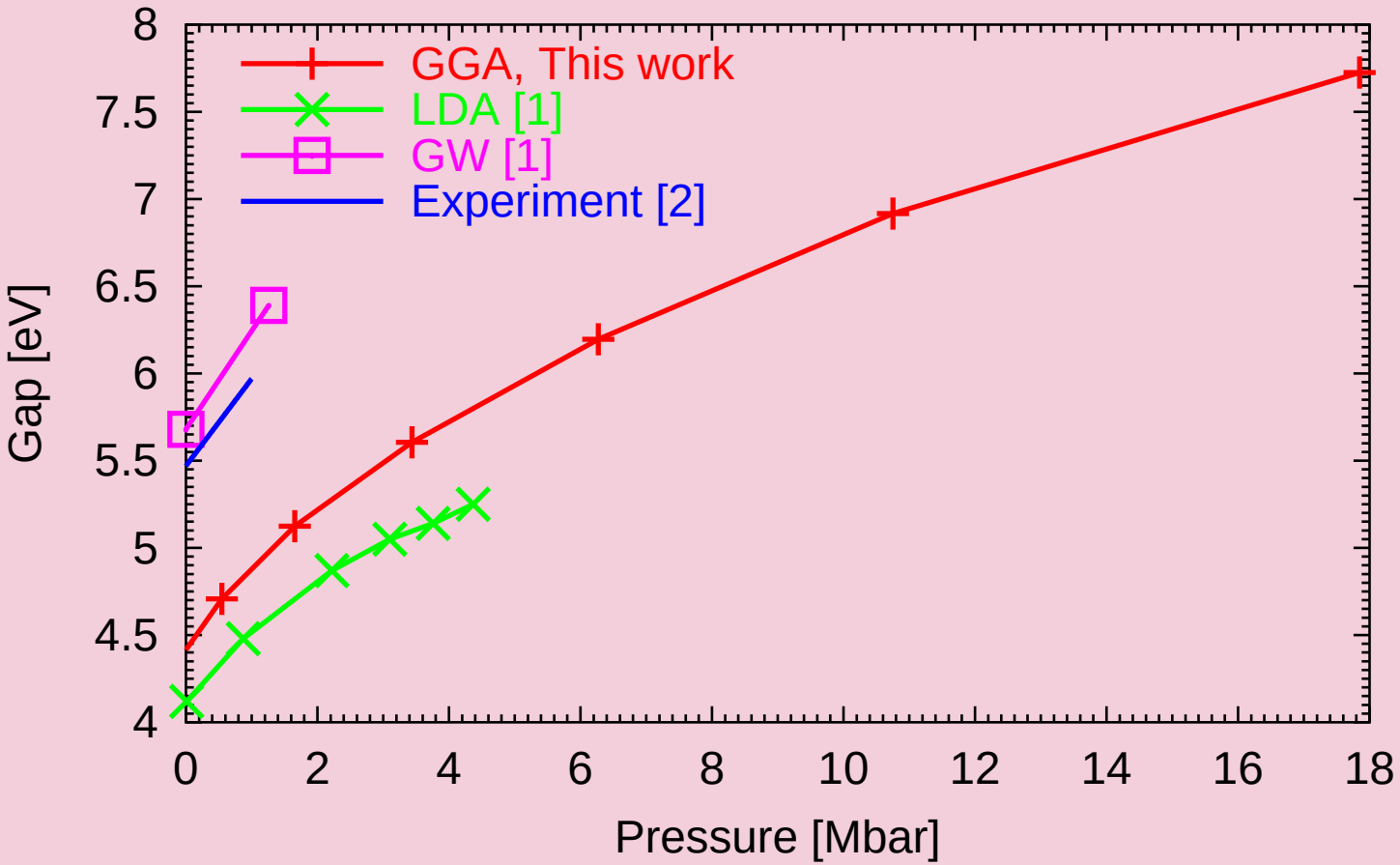
Gap of Diamond increases with Pressure

Gap dependence with Pressure at $T = 0$, Unusual opening of the Gap



[1] Surh et al., PRB 45,8239 (1992)
[2] Dean et al., PRA 140,355 (1965)

Gap Increase with Pressure is determined by Two Factors

1. sp^3 hybridization

- Simple **Bonding-Antibonding picture** works for diamond[5].
- **Silicon** shows opposite behaviour.

2. Symmetry of Diamond structure

- Under **Anisotropic pressure** the gap **decreases**.
- BC8 shows a **decrease** of the gap.
- Thermal disorder produces a **rapid decrease** of the gap.

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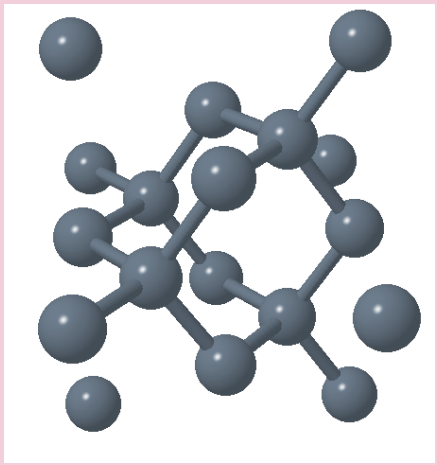
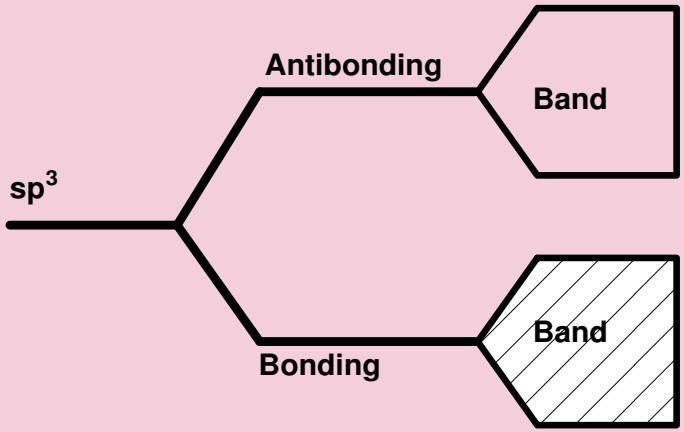
Diamond, Formation of bands





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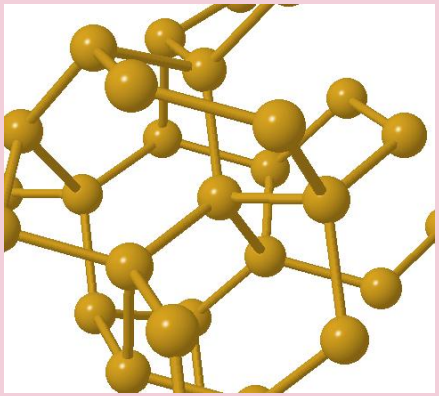
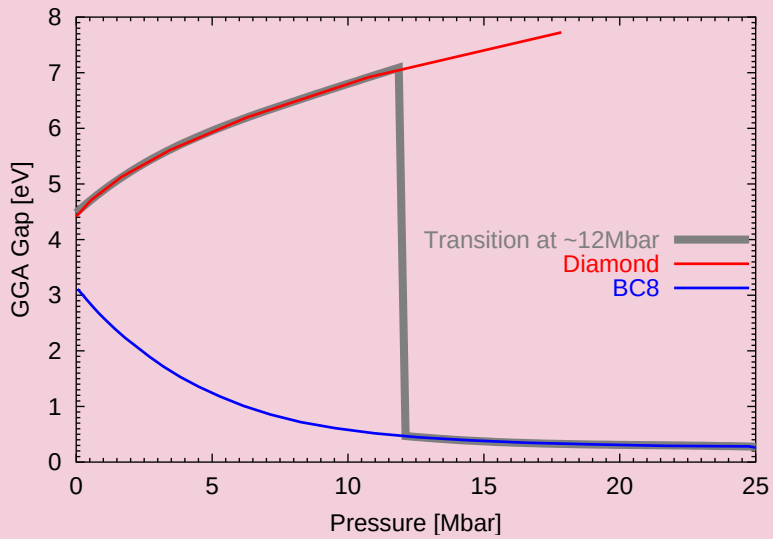
BC8 structure, stable above 12Mbar





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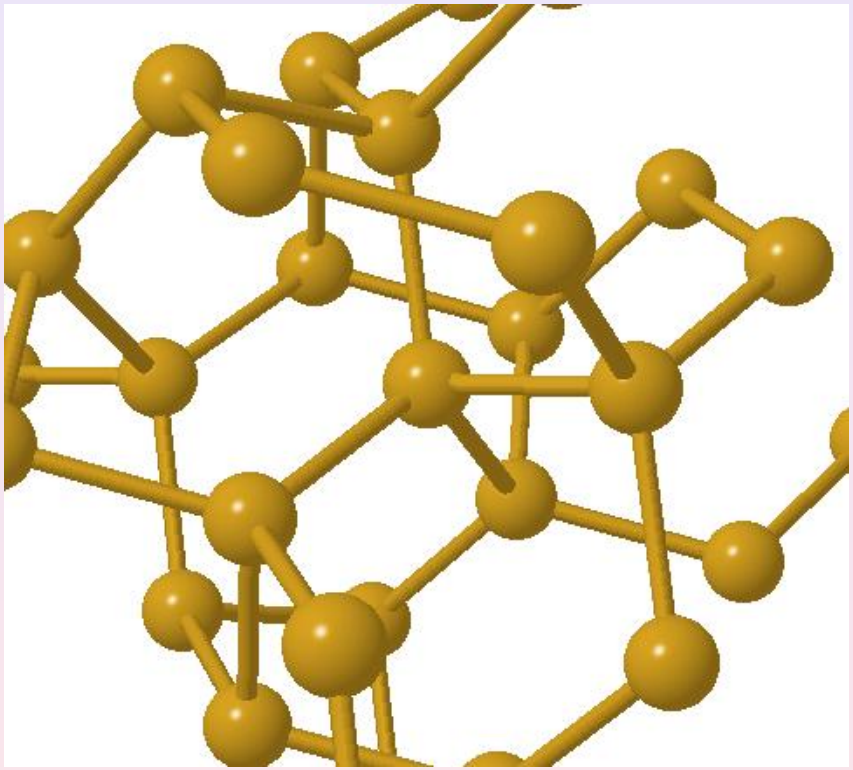
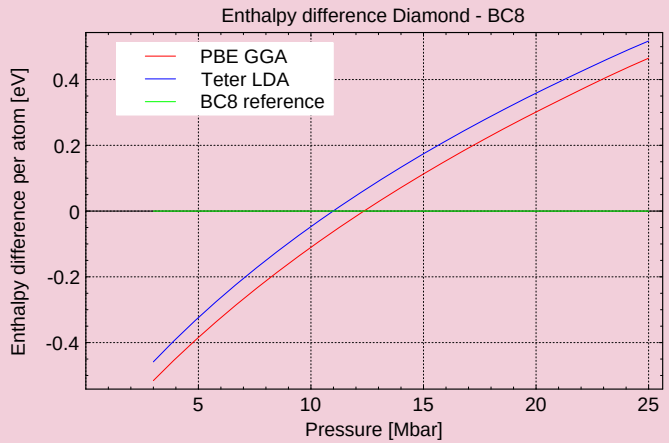
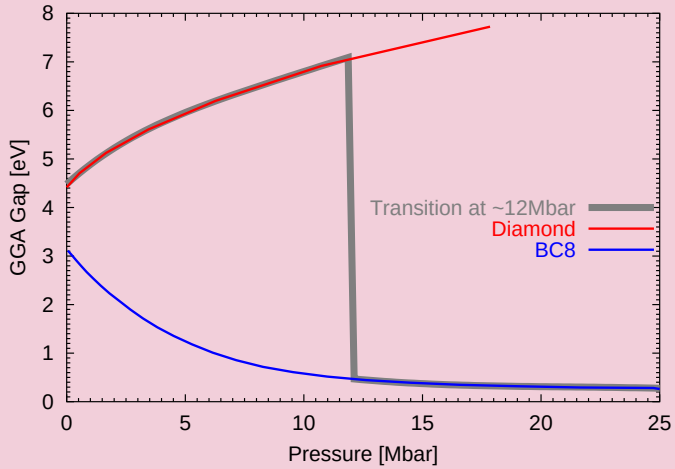
BC8 Structure, 4-fold coord. but different to Diamond



Stable above 12 Mbar, ΔH method



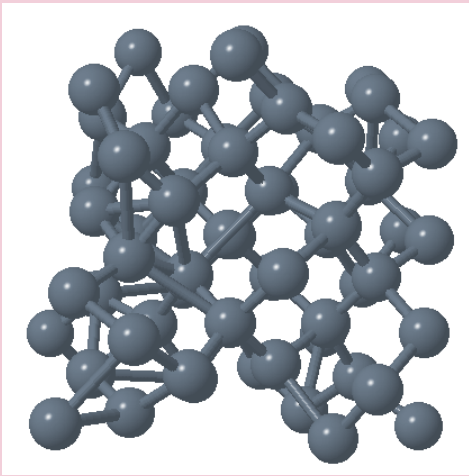
BC8 Gap decreases with Pressure



Gap of Diamond at Finite Temperature: Method

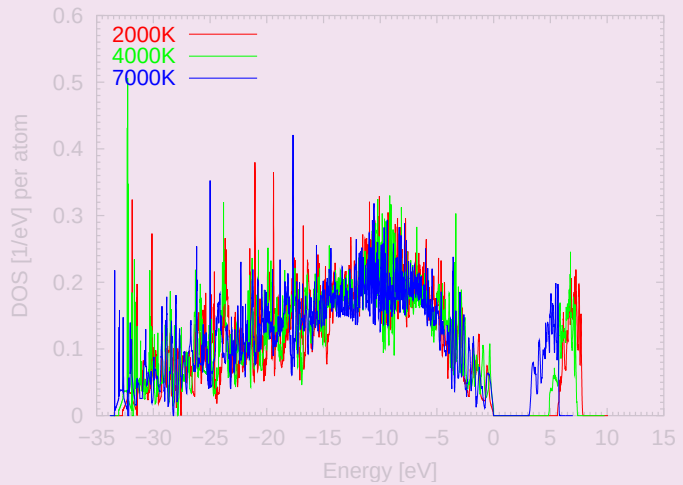
Constant Pressure Molecular Dynamics

- **64 atoms** in a periodic box
- **Car-Parinello** molecular dynamics
- **Norm conserving** pseudo-potential
- Set $P = \sim$10Mbar and $T = 0$ up to 10000K
- $\sim$4 picoseconds **equilibration** time



Density of States

- **DOS** calculated from **Snapshots**
- GGA Energy **Gap** from DOS.



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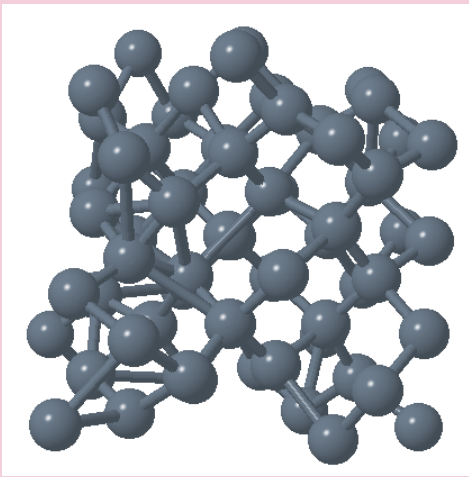

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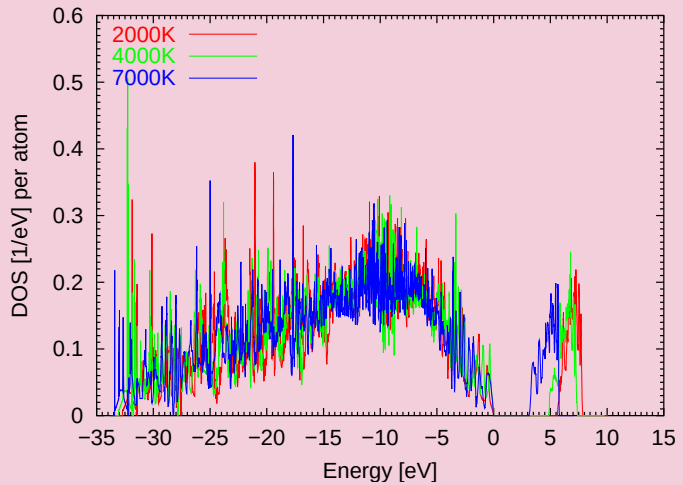
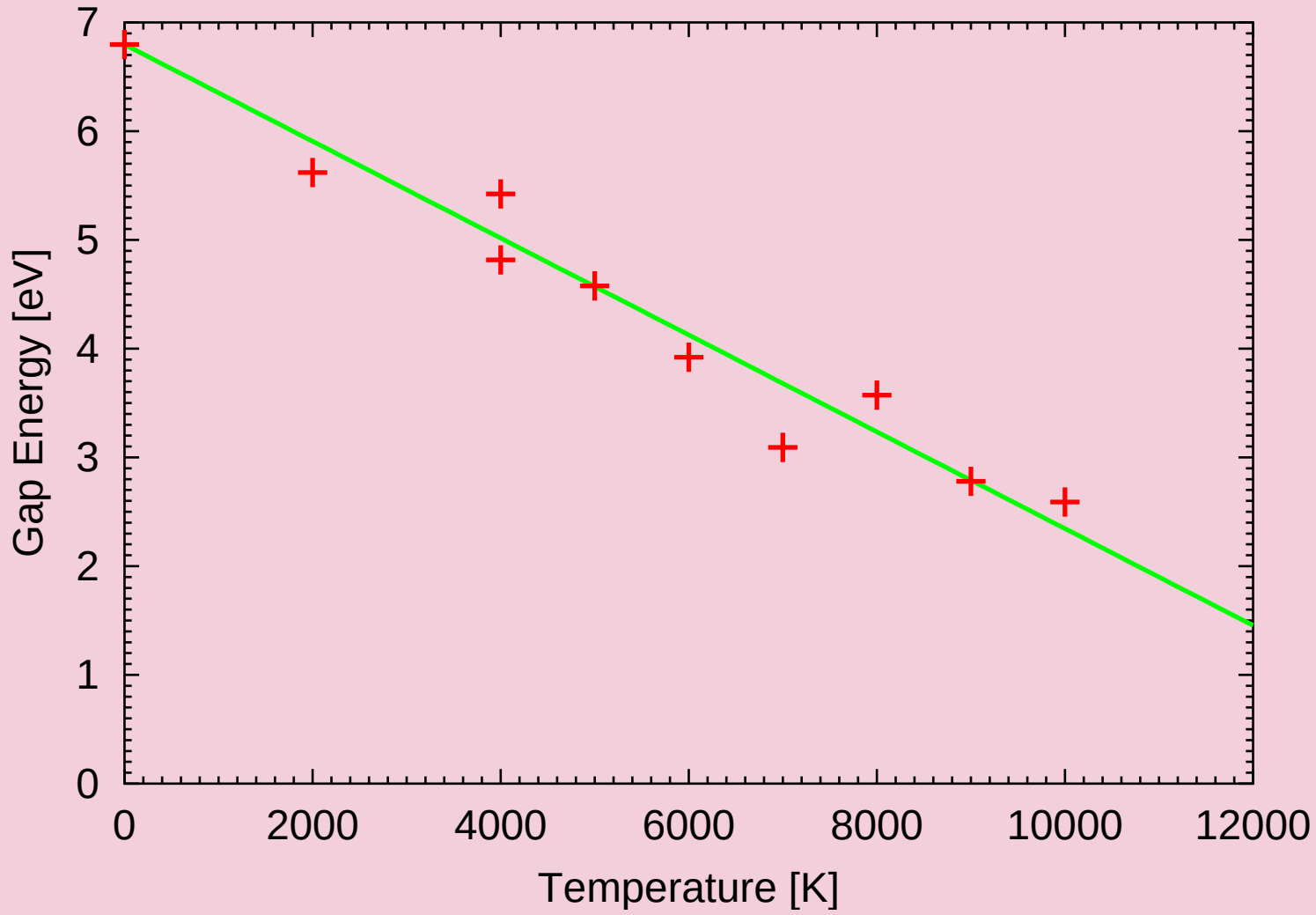


Gap of Diamond reduces with Temperature at High P

Gap dependence with Temperature at $P = 10$ Mbar

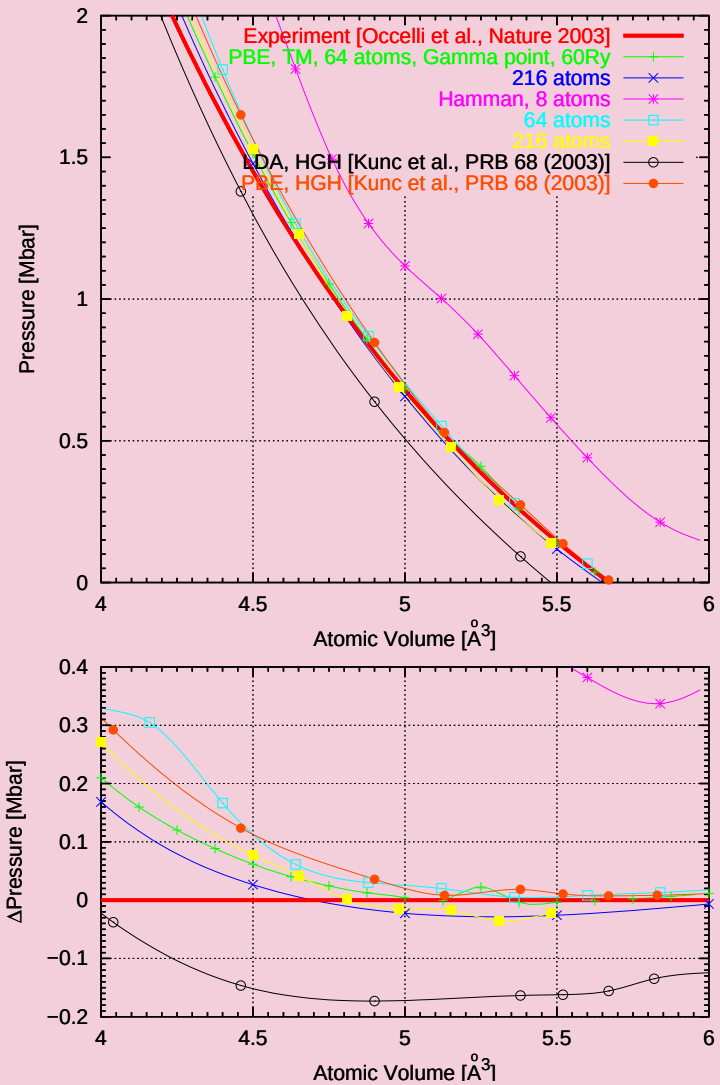


Summary

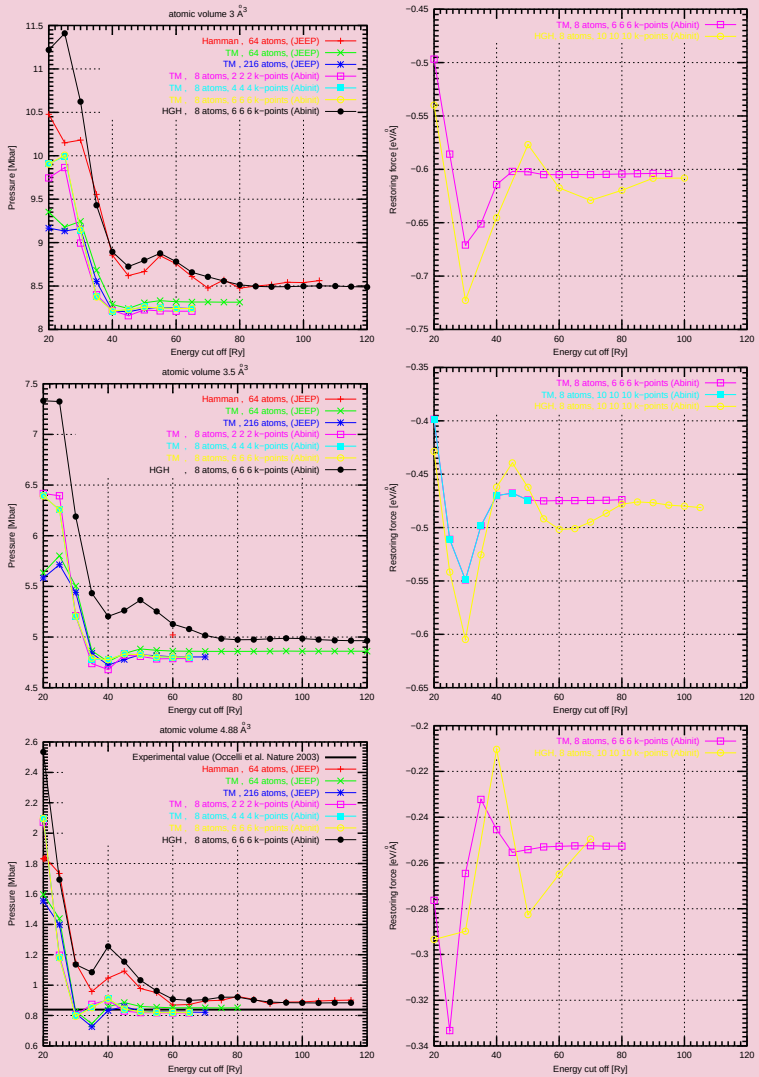
- Energy Gap of Carbon is very sensitive to crystal symmetry.
- BC8 Gap decreases with pressure.
- Diamond Gap increases with pressure.
- but decreases continuously as temperature is raised.
- Diamond at High pressure does not become conducting before melting

Appendix: Convergence tests

Equation of State at $T = 0$, size FX



EOS and forces: Energy cut-off FX



This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.